

(2H)Formaldehyde
1664-98-8 | DTXSID00168098

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 817 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.84e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|---|
| <div>Image not found</div> <div>1,2-Propadiene</div> <div>Measured: 10400</div> <div>Predicted: 1730</div> | <div>Image not found</div> <div>Acetonitrile</div> <div>Measured: 902</div> <div>Predicted: 61.0</div> | <div>Image not found</div> <div>3,3-dichloro-1,1,1,2,2-pentafluoropropane</div> <div>Measured: 63.4</div> <div>Predicted: 483</div> |
| <div>Image not found</div> <div>Propane, 2-iodo-</div> <div>Measured: 1610</div> <div>Predicted: 35.2</div> | <div>Image not found</div> <div>Arecoline</div> <div>Measured: 232</div> <div>Predicted: 1.33e-01</div> | |